Statistical Verification and Validation of the EXFOR Database (A61, A69)

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1. EXFOR checking ("post-SG30" activities)

The Data Bank works to maintain the highest level of quality in its databases.

Verification methods developed within "WPEC Subgroup 30" have been implemented at the Data Bank to further improve the quality of EXFOR:

1.1 In-depth review of all threshold reaction cross-sections

"*Statistical Verification and Validation of the EXFOR database: (n,n'), (n,2n), (n,p), (n,α) and other neutron-induced threshold reaction cross-sections*" by A.Koning, NEA/DB/DOC(2014)3

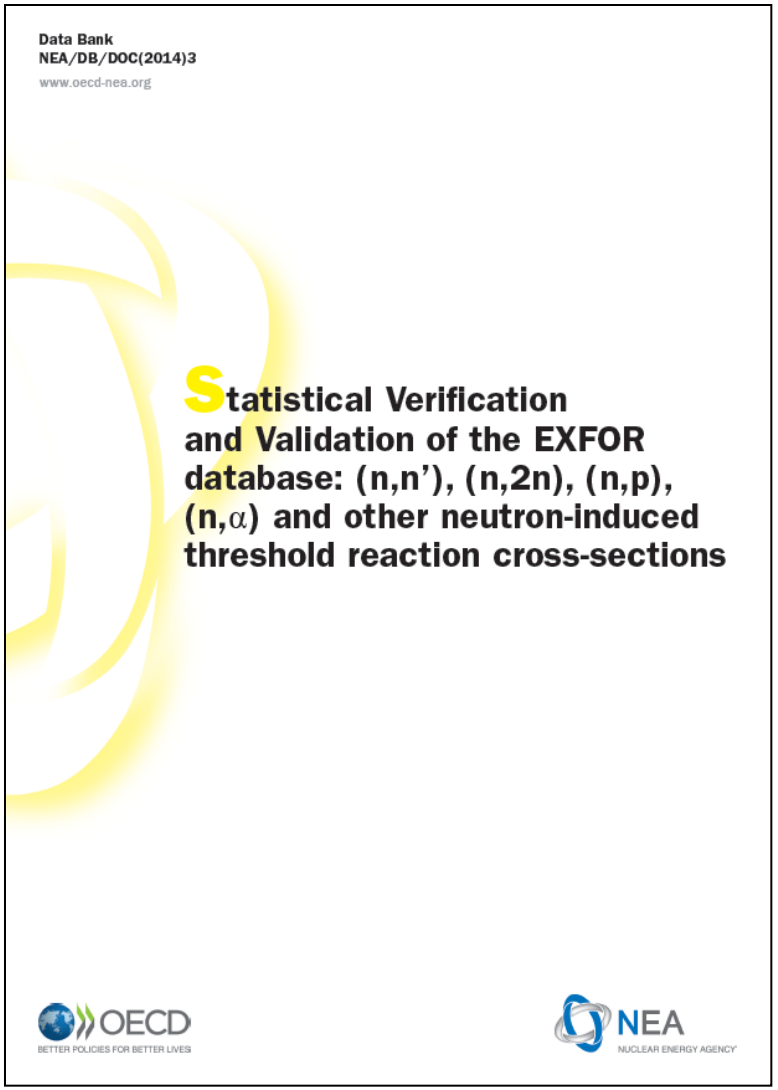
1.2 Implementation of cross-checking with evaluated data

"*Cross-checking of Large Evaluated and Experimental Nuclear Reaction Databases*", by O. Zeydina, A.J. Koning, N. Soppera, D. Raffanel, M. Bossant, E. Dupont, and B. Beauzamy, NDS 120 (2014) 277

1.1 In-depth review of all threshold reaction XSs

An efficient review system and associated strategy were developed to systematically compare more than 10 000 cross-section data sets from EXFOR with the corresponding values in the main evaluated nuclear data libraries, including JEFF.

- The review initially covered all neutron-induced threshold and activation reactions such as (n,n'), (n,2n), (n,p) and (n,α) (NEA, 2014).
- The resulting statistical information showed various **interesting trends in the data**, including a list of **suspicious data sets** for which the cross-section values deviate greatly from the major evaluated nuclear data libraries and/or other measurements.
- The original publications associated with these data have also been systematically checked.



http://www.oecd-nea.org/databank/docs/2014/db-doc2014-3.pdf

Scoring classes… the strongest deviations

T3. Automatically compared with libraries: strong deviations
The subentry contains probably not the reaction and data measured by the author, and the associated publication has not (yet) been checked by the reviewer. **The quantities have central values and uncertainties which are strongly deviating from other measurements, libraries and/or calculations.**

R3. Paper reviewed: strong deviations
The subentry contains certainly the reaction and data measured by the author, since the associated publication has been checked by the reviewer. **The quantities have central values and uncertainties which are strongly deviating from other measurements, libraries and/or calculations.**

E3. Error: subentry contains other quantity or wrong values - strong deviations.
The subentry contains reaction and data that do not agree at all with other measurements, libraries and/or calculations. The associated publication has been checked by the reviewer, and often the values found are wrong. Sometimes, no origin of the value or alternative meaning for the value could be found. **Action: further analysis, confirmation and correction by Data Centres.**

See **WP2013-19**, "*Proposal to introduce a Quality Score in EXFOR",* E. Dupont, A.J. Koning, N. Otsuka

Table. Total number of neutron-induced *cross section* subentries available in XC4 format, compared in this work, and scoring in reviewing classes. EXFOR status: July 7 2014.

Reaction	All	Compared	F < 5	T1	T2	T3	N1	N2	N3	R1	R2	R3	E1	E2	E3	Reviewed
(n,tot)	4528	4421	4390	2187	963	0	816	450	0	0	0	0	0	0	0	
(n,el)	871	852	846	446	225	0	112	67	0	0	0	0	0	0	0	
(n,non)	375	365	364	213	100	0	32	20	0	0	0	0	0	0	0	
(n,n')	229	151	149	52	12	4	49	5	12	6	3	8	0	0	0	y
(n,n')m	255	248	242	57	30	1	92	18	9	16	6	19	0	0	0	y
(n,n')n	3	3	2	0	1	0	0	0	0	0	2	0	0	0	0	y
(n,2n)	1643	1600	1593	378	126	30	331	48	20	408	202	53	2	2	0	y
(n,2n)g	384	377	376	70	20	8	80	24	4	105	35	27	2	0	3	y
(n,2n)m	712	701	691	109	26	6	154	55	5	214	83	47	1	0	2	y
(n,2n)n	42	41	33	7	3	3	5	5	0	3	5	10	0	0	0	y
(n,3n)	94	83	78	17	9	0	34	11	0	6	4	2	0	0	0	y
(n,3n)g	8	6	4	3	0	0	0	3	0	0	0	0	0	0	0	y
(n,3n)m	19	16	16	6	4	0	1	4	0	1	0	0	0	0	0	y
(n,f)	1229	1153	1127	515	131	112	267	68	56	0	0	0	0	0	0	
(n,na)	53	53	36	23	9	0	4	2	0	9	6	0	0	0	0	y
(n,na)g	1	1	1	1	0	0	0	0	0	0	0	0	0	0	0	y
(n,na)m	15	14	12	3	1	0	1	2	0	7	0	0	0	0	0	y
(n,na)n	4	4	4	1	0	0	1	0	0	2	0	0	0	0	0	y
(n,2na)	20	5	5	2	3	0	0	0	0	0	0	0	0	0	0	y
(n,np)	75	196	136	52	12	0	60	41	0	21	9	1	0	0	0	y
(n,np)g	5	16	11	3	1	0	7	2	0	2	1	0	0	0	0	y
(n,np)m	16	62	45	12	5	0	20	16	0	8	1	0	0	0	0	y
(n,n2a)	8	8	8	3	0	0	5	0	0	0	0	0	0	0	0	y
(n,nd)	6	6	5	3	0	1	1	0	0	0	1	0	0	0	0	y
(n,nt)	28	1	0	0	1	0	0	0	0	0	0	0	0	0	0	y
(n,4n)	34	32	32	8	4	0	10	7	0	3	0	0	0	0	0	y
(n,4n)g	3	3	3	1	0	0	2	0	0	0	0	0	0	0	0	y
(n,2np)	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	y
(n,n'$_1$)	726	337	317	170	24	1	112	9	7	6	1	6	0	0	1	y
(n,n'$_2$)	0	105	96	51	14	2	28	6	2	0	2	0	0	0	0	y
(n,n'$_3$)	0	44	31	14	8	1	12	8	1	0	0	0	0	0	0	y
(n,n'$_4$)	0	25	17	9	10	0	2	4	0	0	0	0	0	0	0	y
(n,n'$_5$)	0	18	16	12	2	0	1	1	0	1	0	1	0	0	0	y
(n,n'$_6$)	0	17	15	5	6	0	3	3	0	0	0	0	0	0	0	y
(n,n'$_{>6}$)	0	65	42	15	28	0	9	13	0	0	0	0	0	0	0	y

Reaction	All	Compared	F < 5	T1	T2	T3	N1	N2	N3	R1	R2	R3	E1	E2	E3	Reviewed
(n,abs)	156	25	17	6	7	7	1	3	1	0	0	0	0	0	0	y
(n,g)	5360	5282	4970	2590	426	734	984	195	333	0	0	0	0	0	0	
(n,g)g	339	325	298	150	27	26	70	25	23	0	0	0	0	0	0	
(n,g)m	549	543	461	248	78	27	116	54	15	0	0	0	0	0	0	
(n,g)n	28	22	16	2	6	1	4	9	0	0	0	0	0	0	0	
(n,p)	1835	1817	1771	469	144	22	296	91	11	483	288	9	1	2	1	y
(n,p)g	198	193	179	35	6	0	42	13	0	59	33	1	0	4	1	y
(n,p)m	438	434	410	81	20	0	68	44	0	146	71	0	1	4	0	y
(n,p)n	12	12	9	0	1	0	1	5	0	4	1	0	0	0	0	y
(n,d)	33	32	29	13	8	0	4	5	0	1	1	0	0	0	0	y
(n,d)g	1	1	1	0	1	0	0	0	0	0	0	0	0	0	0	y
(n,d)m	3	3	2	0	0	0	0	3	0	0	0	0	0	0	0	y
(n,t)	147	138	127	59	18	0	31	20	0	3	7	2	0	0	0	y
(n,t)g	21	7	3	1	5	0	0	1	0	0	0	0	0	0	0	y
(n,t)m	26	19	14	0	15	0	1	3	0	0	0	1	0	0	0	y
(n,t)n	1	1	0	0	0	0	0	1	0	0	0	0	0	0	0	y
(n,h)	60	15	5	4	1	0	4	4	0	2	0	5	0	0	0	y
(n,h)m	6	4	4	4	0	0	0	0	0	0	0	1	0	0	0	y
(n,a)	1119	1103	1035	346	118	12	181	64	3	223	149	6	2	0	1	y
(n,a)g	87	86	75	24	4	0	11	3	0	23	21	0	0	0	0	y
(n,a)m	209	208	189	41	15	0	40	10	0	61	41	0	0	0	0	y
(n,a)n	1	1	0	0	0	0	0	1	0	0	0	0	0	0	0	y
(n,2a)	5	5	4	0	4	0	1	0	0	0	0	0	0	0	0	y
(n,2p)	34	5	1	0	4	0	0	0	0	1	0	9	0	0	0	y
(n,2p)m	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	y
(n,pa)	6	5	5	1	0	0	1	2	0	1	0	0	0	0	0	y
(n,t2a)	2	2	1	0	0	0	1	1	0	0	0	0	0	0	0	y
(n,xn)	17	12	10	2	2	0	2	1	0	3	0	2	0	0	0	y
(n,xg)	690	527	325	26	128	151	9	80	133	0	0	0	0	0	0	y
(n,xg)m	15	0	0	0	0	0	0	0	0	0	0	0	0	0	0	y
(n,xp)	89	54	51	16	8	0	12	4	3	5	2	4	0	0	0	y
(n,xd)	23	7	5	1	2	0	4	0	0	0	0	0	0	0	0	y
(n,xt)	37	22	20	10	6	1	4	0	0	0	0	1	0	0	0	y
(n,xh)	9	3	1	0	1	0	1	1	0	0	0	0	0	0	0	y
(n,xa)	165	135	124	66	23	7	19	15	1	2	1	1	0	0	0	y
(n,x)	326	157	145	83	31	0	27	14	0	2	0	0	0	0	0	y
(n,x)g	24	9	9	4	4	0	1	0	0	0	0	0	0	0	0	y
(n,x)m	96	25	22	13	8	1	0	1	2	0	0	0	0	0	0	y
(n,x)n	3	1	1	1	0	0	0	0	0	0	0	0	0	0	0	y
Total	23541	22271	21084	8744	2899	1158	4187	1567	641	1864	988	216	9	14	9	

1.1 In-depth review of all threshold reaction XSs

This work has showed:

- Most of the experimental data were compiled correctly in the EXFOR database
- Few compilation mistakes (that have since been corrected)

On going and future work:

- A second part of the review devoted to the (n, γ) cross-section.
  This part of the review is challenging because of the large fluctuations of data in the resonance region that make the comparison more difficult.

- Other non-threshold cross-sections such as (n,f), (n,tot) and (n,n).

1.2 Cross-checking with evaluated data

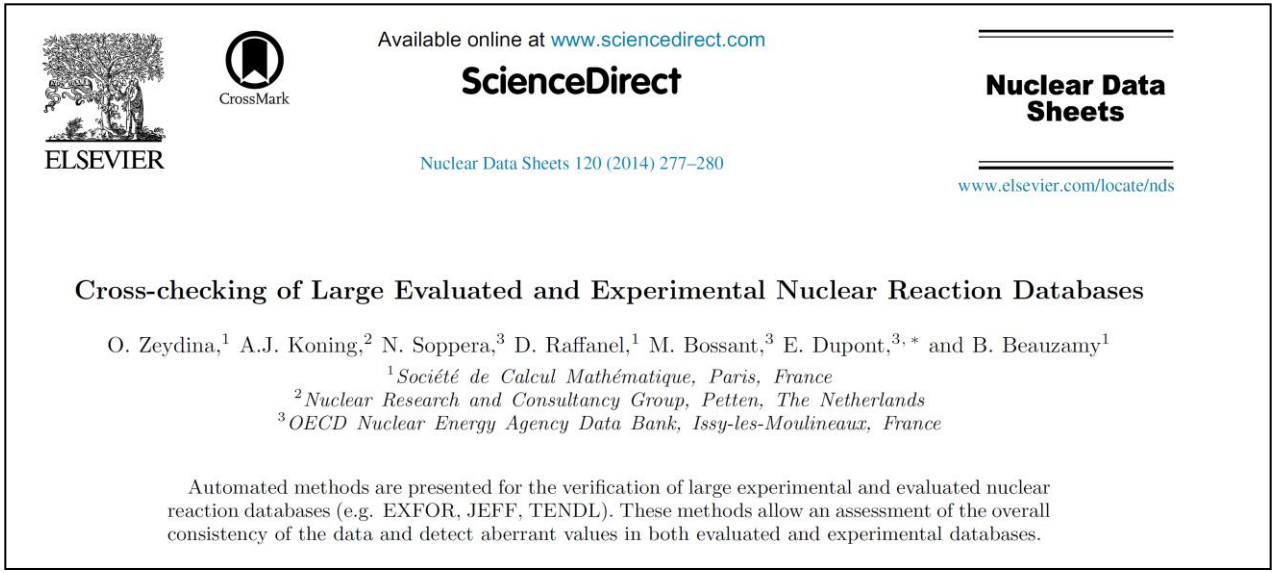
Method developed to cross check evaluated and experimental data in databases in order to detect aberrant values.

- **Methodology**

  Based on distances/ranking of EXFOR-ENDF and ENDF-ENDF

- **Outliers**

  "There is no evidence, on the basis of numerical comparisons only, that **outliers** represent "bad" data"



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Cross-checking of Large Evaluated and Experimental Nuclear Reaction Databases

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Automated methods are presented for the verification of large experimental and evaluated nuclear reaction databases (e.g. EXFOR, JEFF, TENDL). These methods allow an assessment of the overall consistency of the data and detect aberrant values in both evaluated and experimental databases.

- **Helping ND evaluators**

  "The fact that such data deviate significantly from other data of the same reaction may, however, be **helpful to nuclear data evaluators** who focus on one or a few isotopes and may wish to discard such data after a thorough analysis"

SCM: ENDF-EXFOR method

- **ENDF-ENDF method**: “The absolute distance between the two libraries describing the same reaction is calculated as the integral of the difference between continuous functions. The relative one is deduced by dividing the absolute difference by the average of compared values. The final mean distance is the average of mutual distances.

- **ENDF-EXFOR method**: The absolute distance between a curve and a set of points is taken as the average of all differences of two cross-sections corresponding to the same abscissa (energy).

- **Classification of nuclear reactions**: in order to rate available nuclear reactions according to quality of their representation, a special indicator, combining the absolute and relative distances is implemented:

$$Ind = (log_{10}\, abs)^{norm} \times rel$$

- **Remark:** this indicator is able to rate the reactions only between themselves, that is to indicate the best and the worst representation among the considered ones.

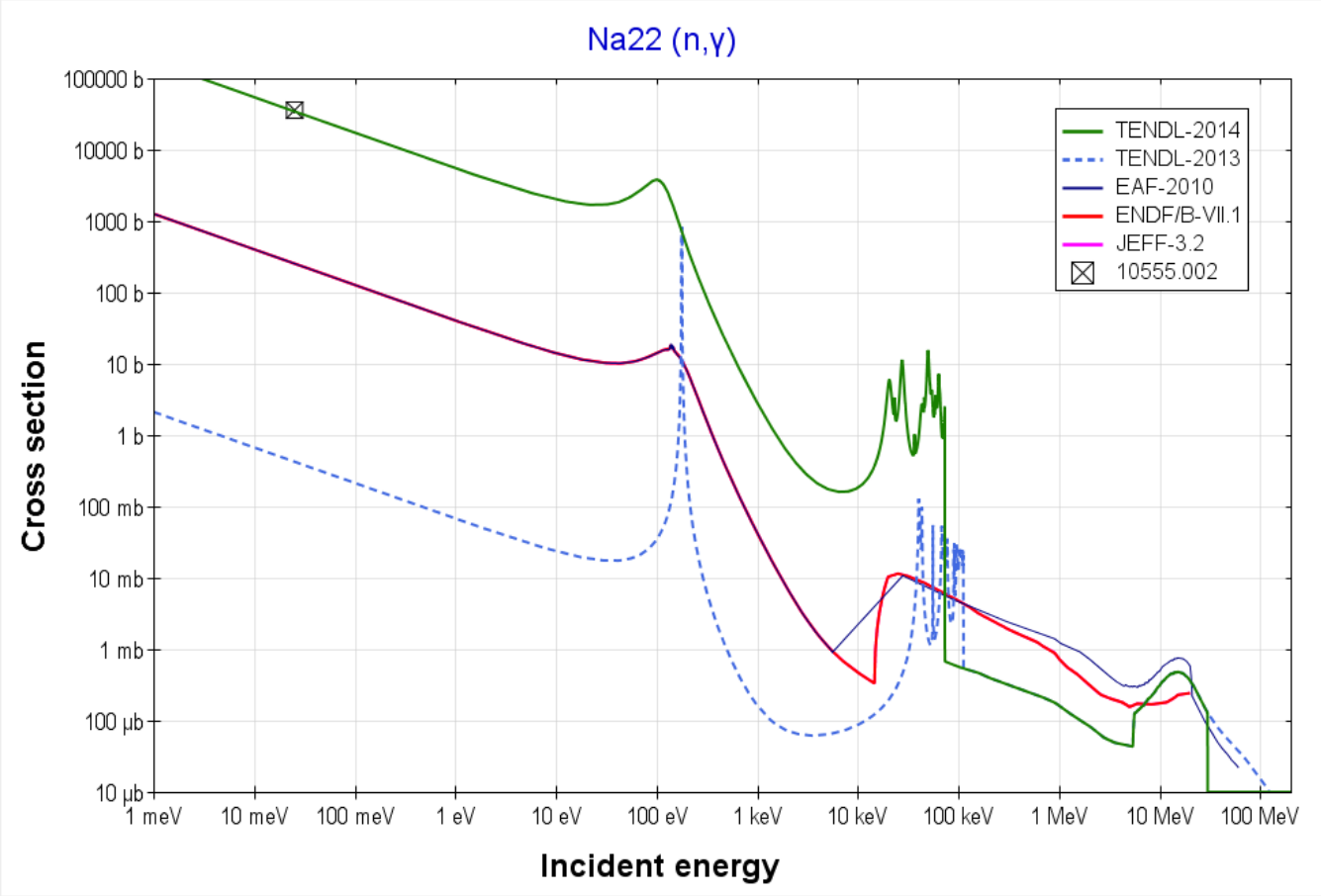
Table 1. Ranking analysis about data quality

quantile	Reaction title	Rank	Evaluated data	Experimental data
q100	11-NA-22(N,G)11-NA-23,,SIG (1,5) E	1,92	TENDL-13	(1 point)
q100	91-PA-234(N,F),,SIG (1,2) E	1,77		(1 point)
q100	3-LI-6(N,G)3-LI-7,,SIG (2,7) E	1,68		
q100	79-AU-198(N,TOT),,SIG (1,1) E	1,65	(1 libr.)	(1 point)
q100	71-LU-177-M(N,G)71-LU-178-M,,SIG (1,3) E	1,61		(1 point)
q100	45-RH-105(N,G)45-RH-106-M,,SIG,,,RECOM (1,1) E	1,59	(1 libr.)	(1 point)
q100	99-ES-253(N,G)99-ES-254-G,,SIG,,,RECOM (1,6) E	1,48		(1 point)
q100	10-NE-21(N,A)8-O-18,,SIG (1,4) E	1,47		(1 point)
q100	68-ER-170(N,G)68-ER-171,,SIG,,,CALC (1,6) E	1,45	(EAF-10)	(1 point)
q100	80-HG-200(N,G)80-HG-201,,SIG,,,RECOM (1,7) E	1,40	TENDL-13	(1 point)
q100	18-AR-39(N,A)16-S-36,,SIG,,,RECOM (1,4) E	1,40		(1 point)
q100	47-AG-110-M(N,G)47-AG-111,,SIG,,,RECOM (1,1) E	1,38	(1 libr.)	(1 point)
q100	95-AM-243(N,G)95-AM-244-G,,SIG,,,RECOM (1,7) E	1,36		(1 point)
q99	96-CM-248(N,G)96-CM-249,,SIG (1,6) E	1,03		
q99	48-CD-106(N,D)47-AG-105,,SIG (1,5) E	1,02		(1 point)
q95	50-SN-0(N,G),,SIG,,,DERIV (8,2) E	0,653		
q95	52-TE-122(N,G)52-TE-123,,SIG (5,6) E	0,653		(1 point)
q90	8-O-17(N,A)6-C-14,,SIG (2,5) E	0,46		

Reactions (n,gamma)

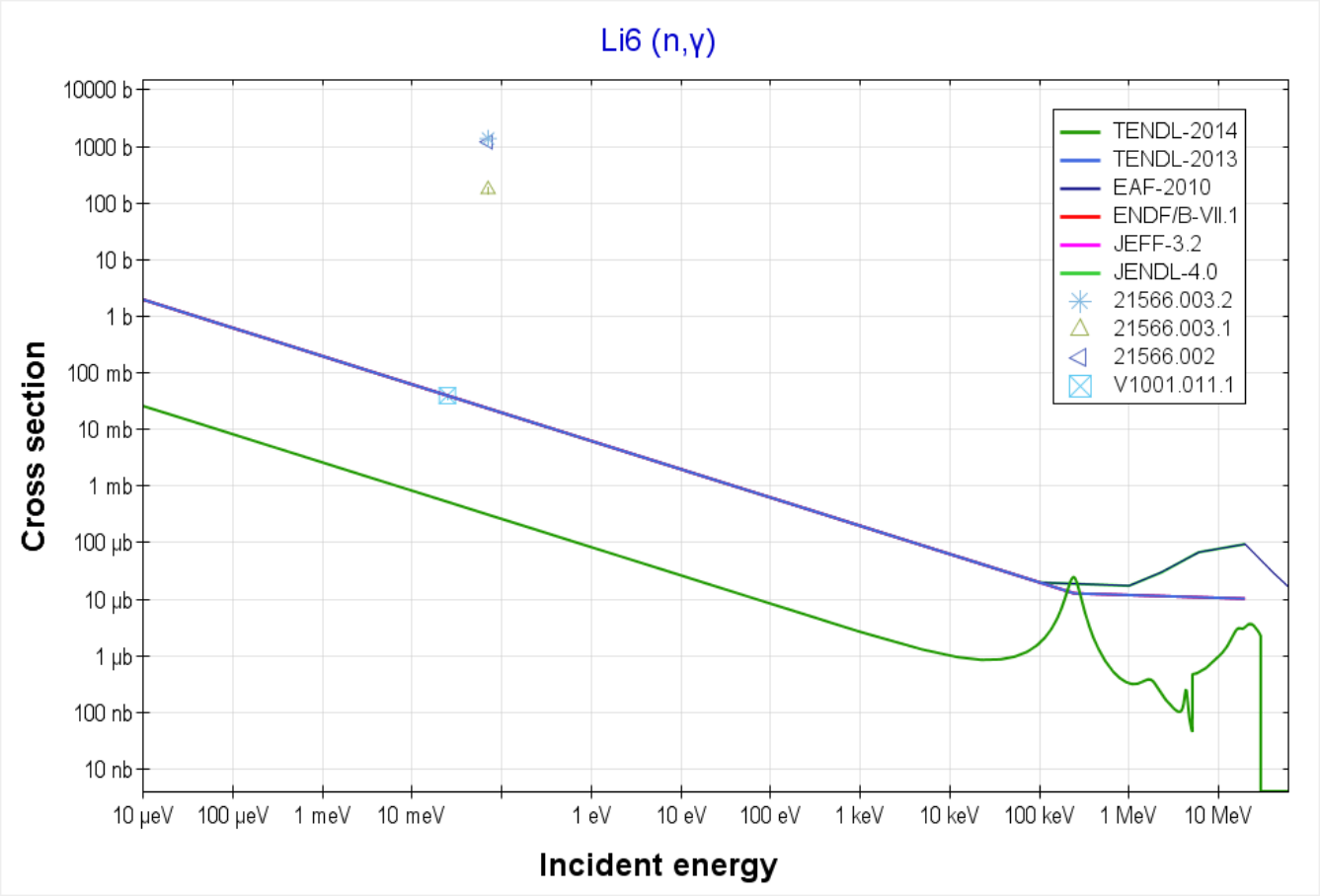
- **Figure.** Na22(n,g) rank value=1.92
- **Figure.** Li6(n,g) rank value=1.68
- **Figure.** Lu177-M(n,g)Lu178-M rank value=1.61
- **Figure.** Rh105(n,g)Rh106-M rank value=1.59
- **Figure.** Es253(n,g)Es-254G rank value=1.48
- **Figure.** Es253(n,g)Es-254G rank value=1.48
- **Figure.** Sn-nat(n,g) rank value=0.653
- **Figure.** Ba130(n,g)

Figure. Na22(n,g) rank value=1.92



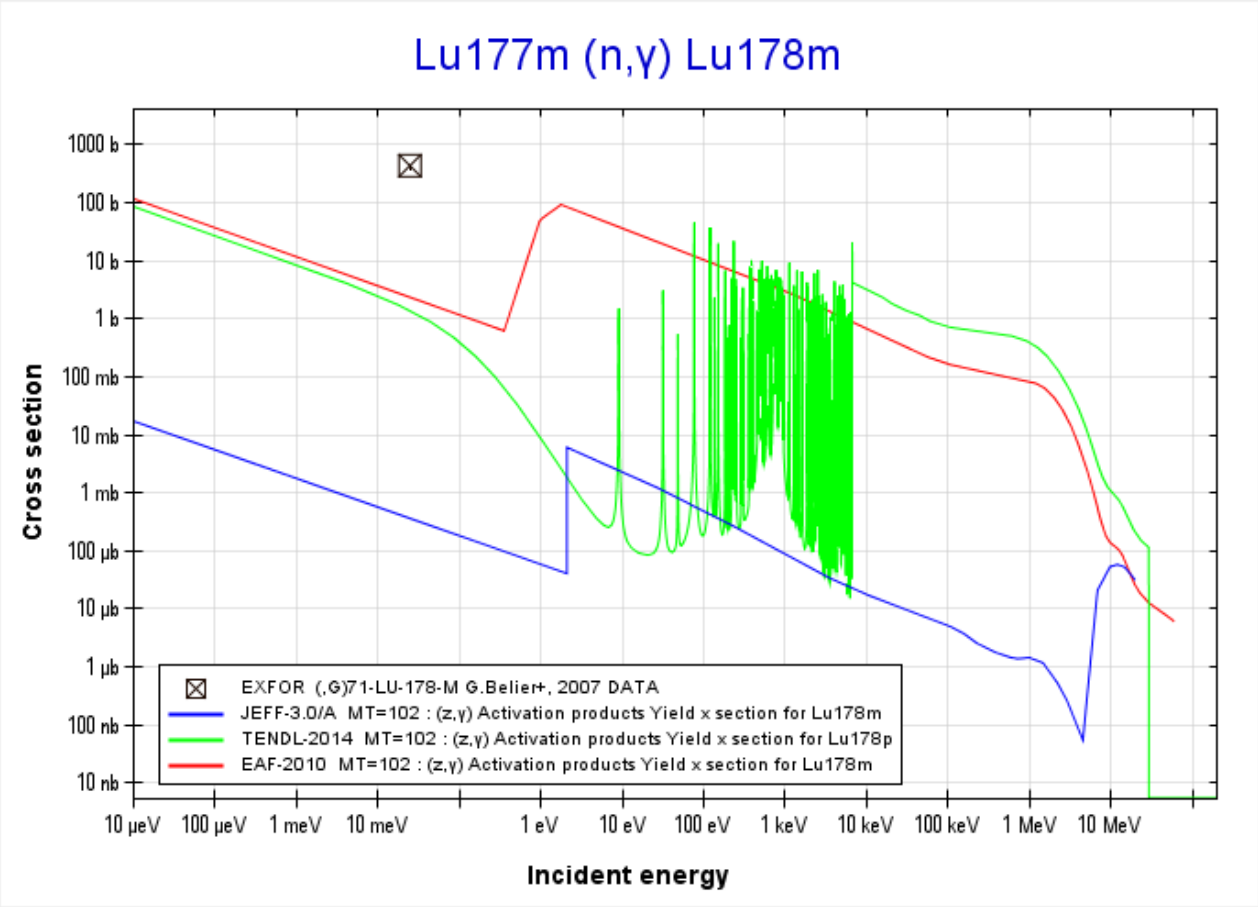
- New evaluations (e.g.TENDL-2014)

Figure. Li6(n,g) rank value=1.68



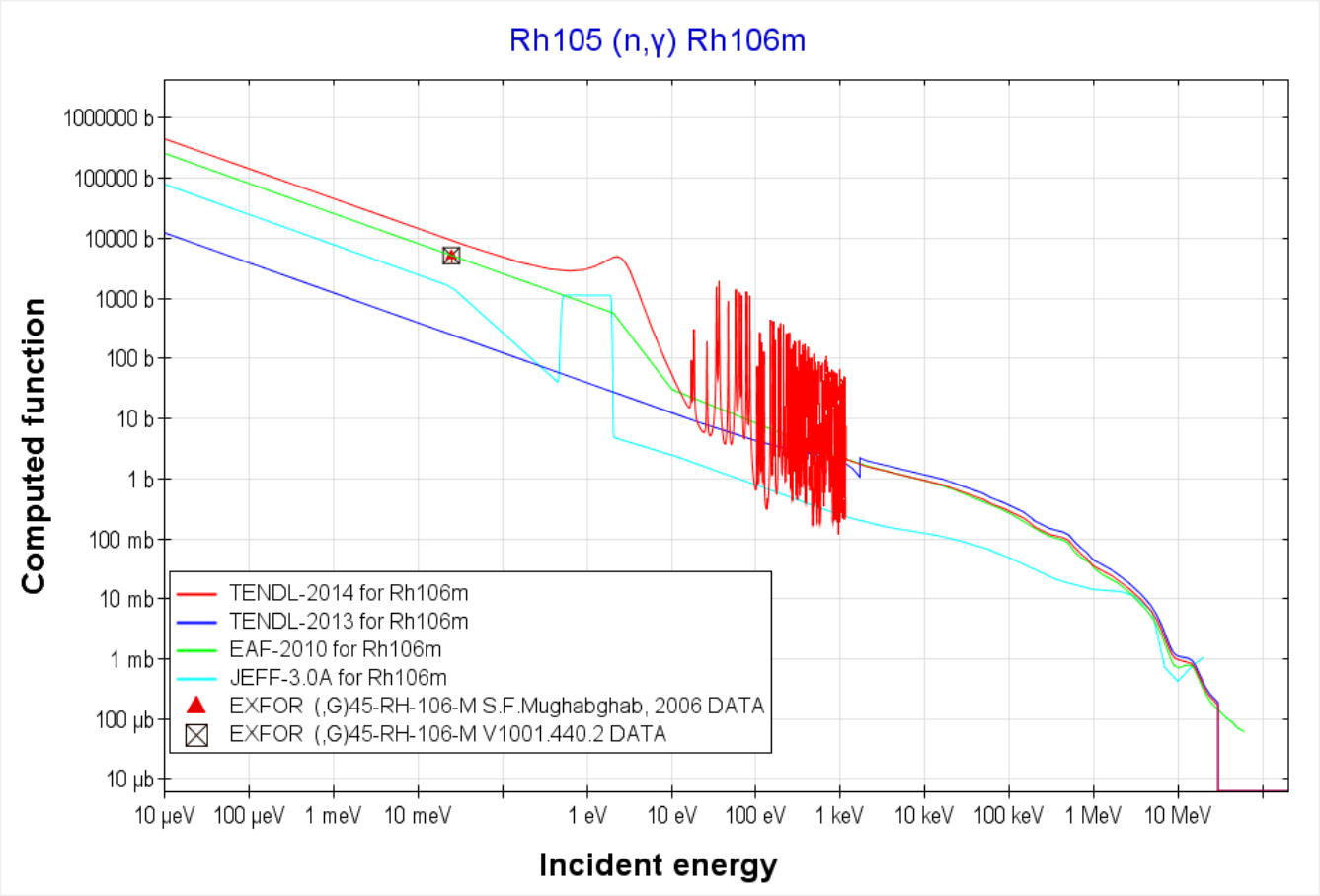
➢ Large disagreement in EXFOR data

Figure. Lu177-M(n,g)Lu178-M rank value=1.61



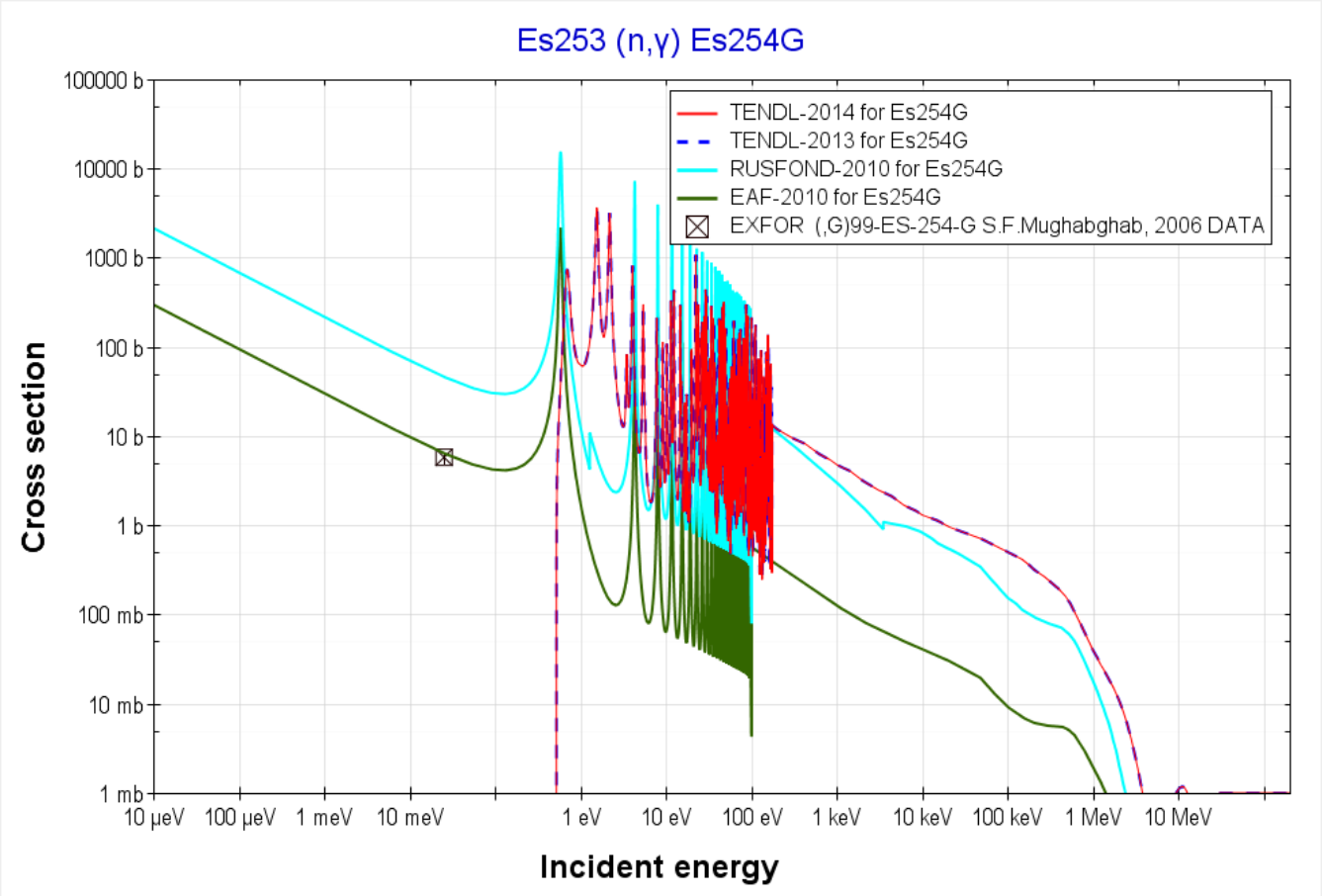
- EXFOR data for isomeric isotopes

Figure. Rh105(n,g)Rh106-M rank value=1.59



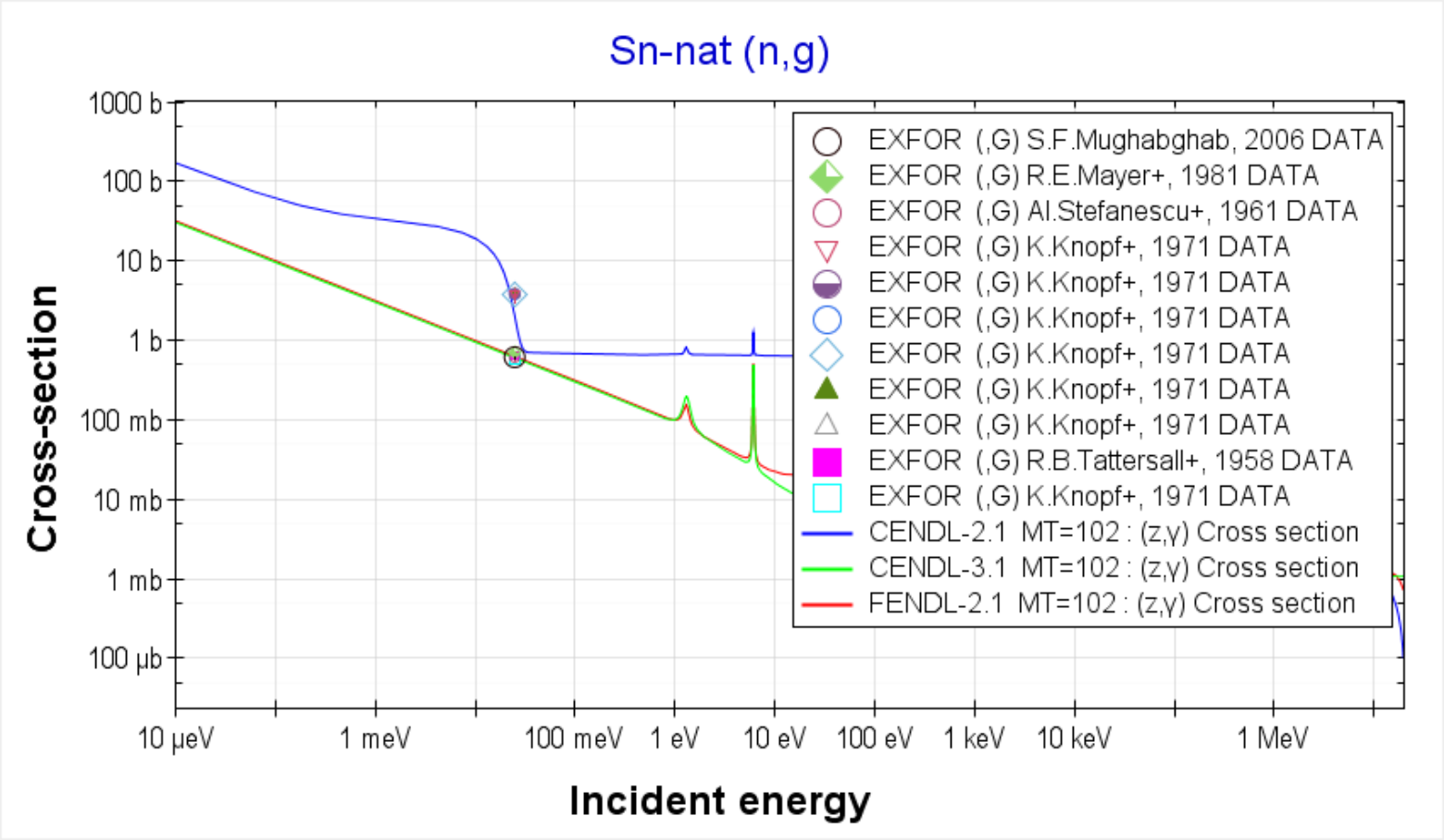
- EXFOR data for isomeric reactions

Figure. Es253(n,g)Es-254G rank value=1.48



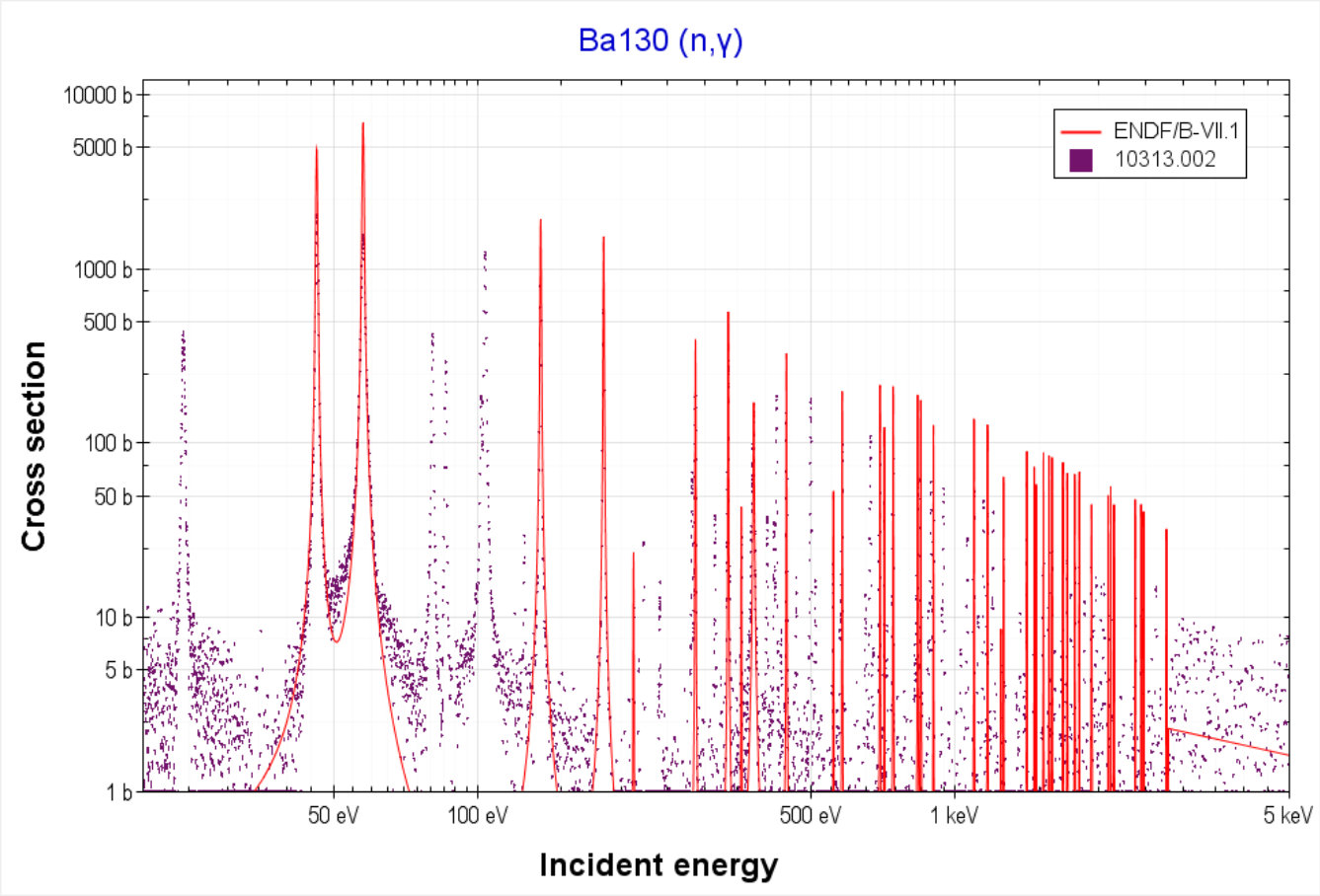
- EXFOR data for isomeric reactions (Ground-Meta)

Figure. Sn-nat(n,g) rank value=0.653



- EXFOR for natural elements

Figure. Ba130(n,g)

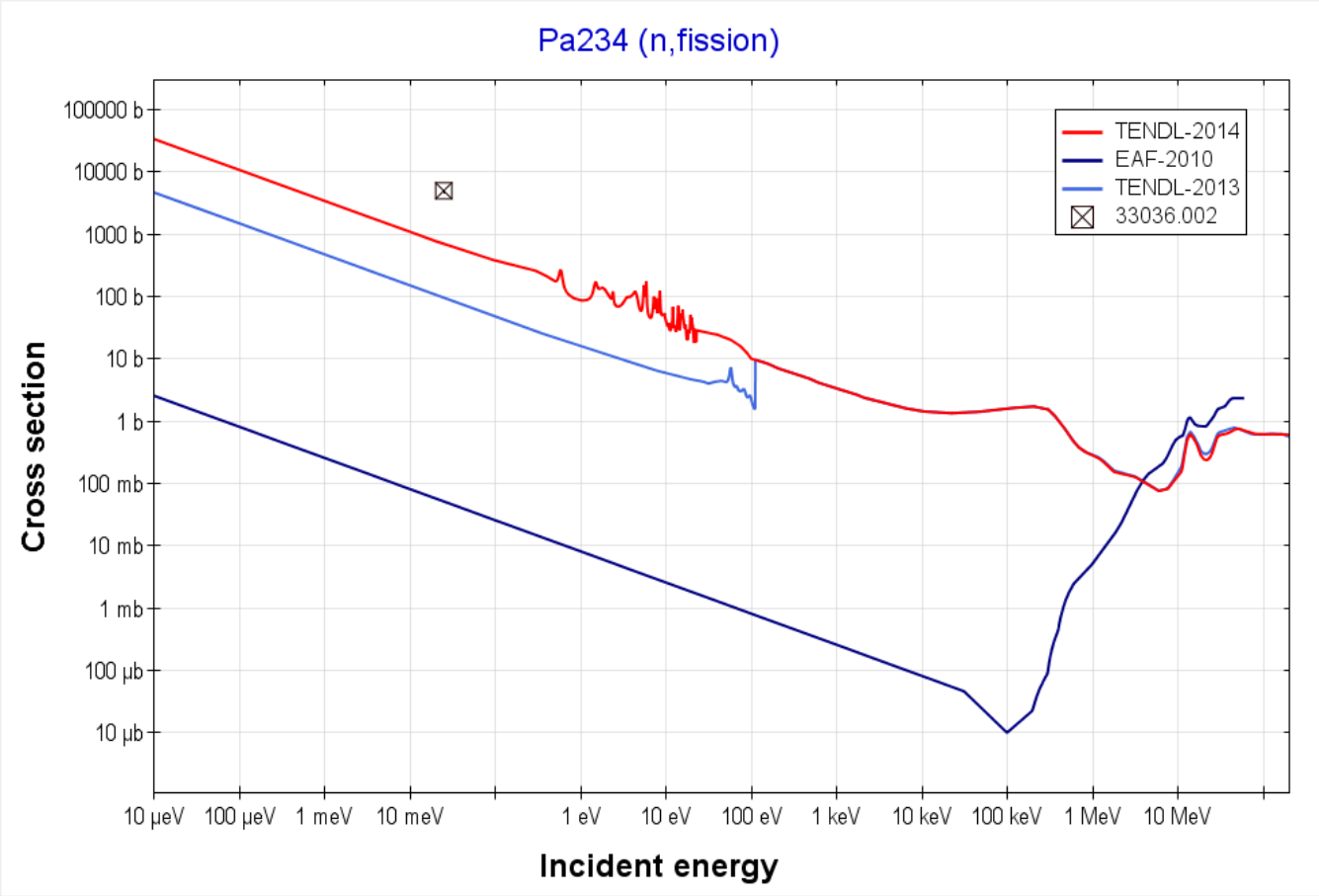


- EXFOR data for improving RRR evaluation

Reactions (n,fission)

- **Figure.** Pa234(n,fission) rank value=1.77

Figure. Pa234(n,fission) rank value=1.77

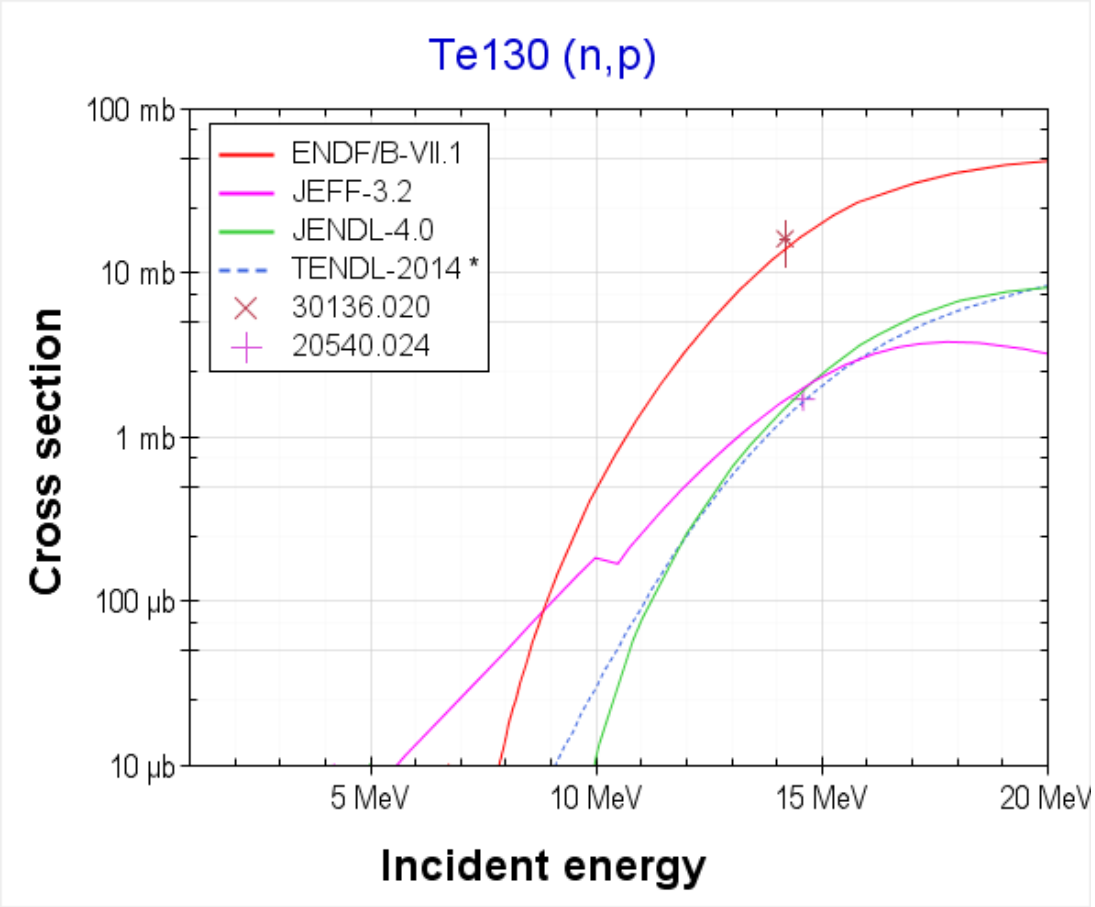


➢ EXFOR data to be used…

Reactions (n,p)

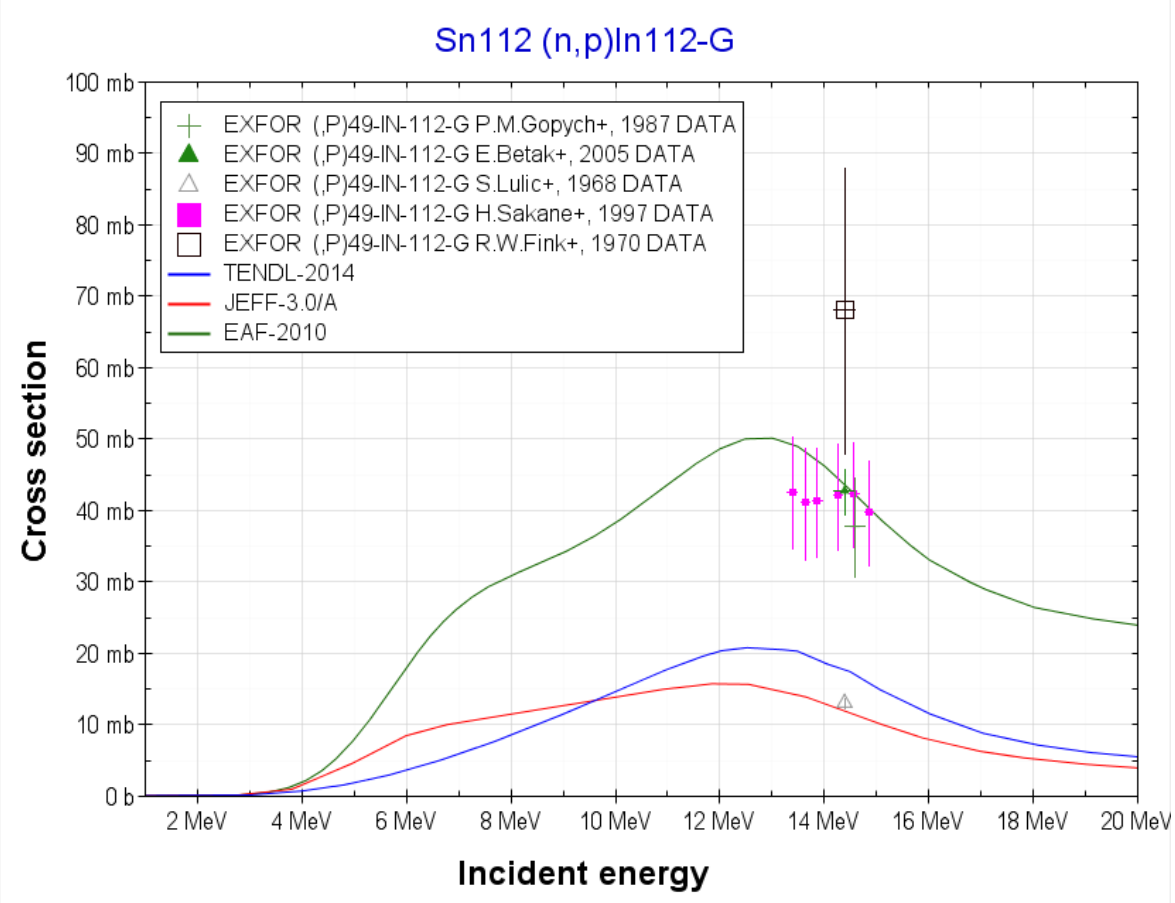
- **Figure.** Te130 (n,p)
- **Figure.** Sn112 (n,p) In112-G

Figure. Te130 (n,p)



- EXFOR data for activation at 14 MeV

Figure. Sn112 (n,p) In112-G

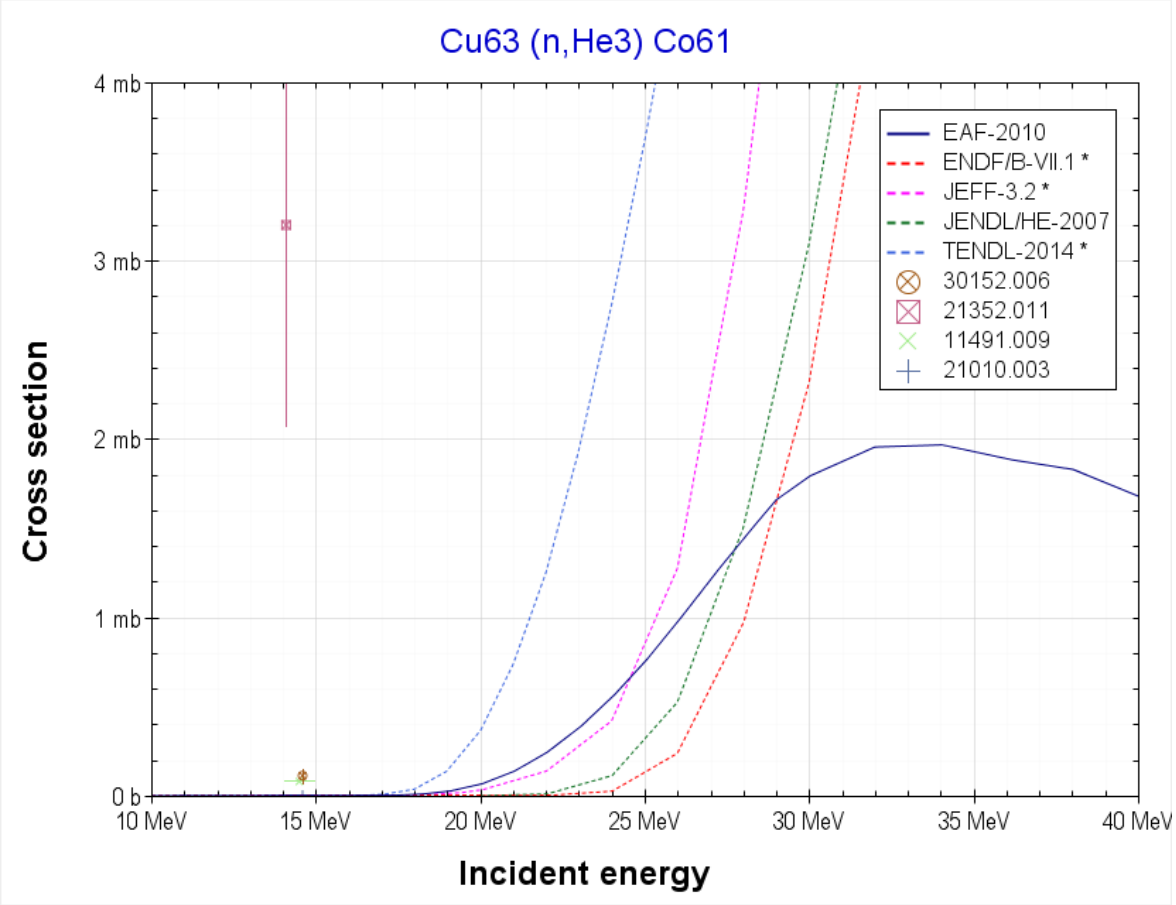


- EXFOR data for activation at 14 MeV

Reactions (n,He3)

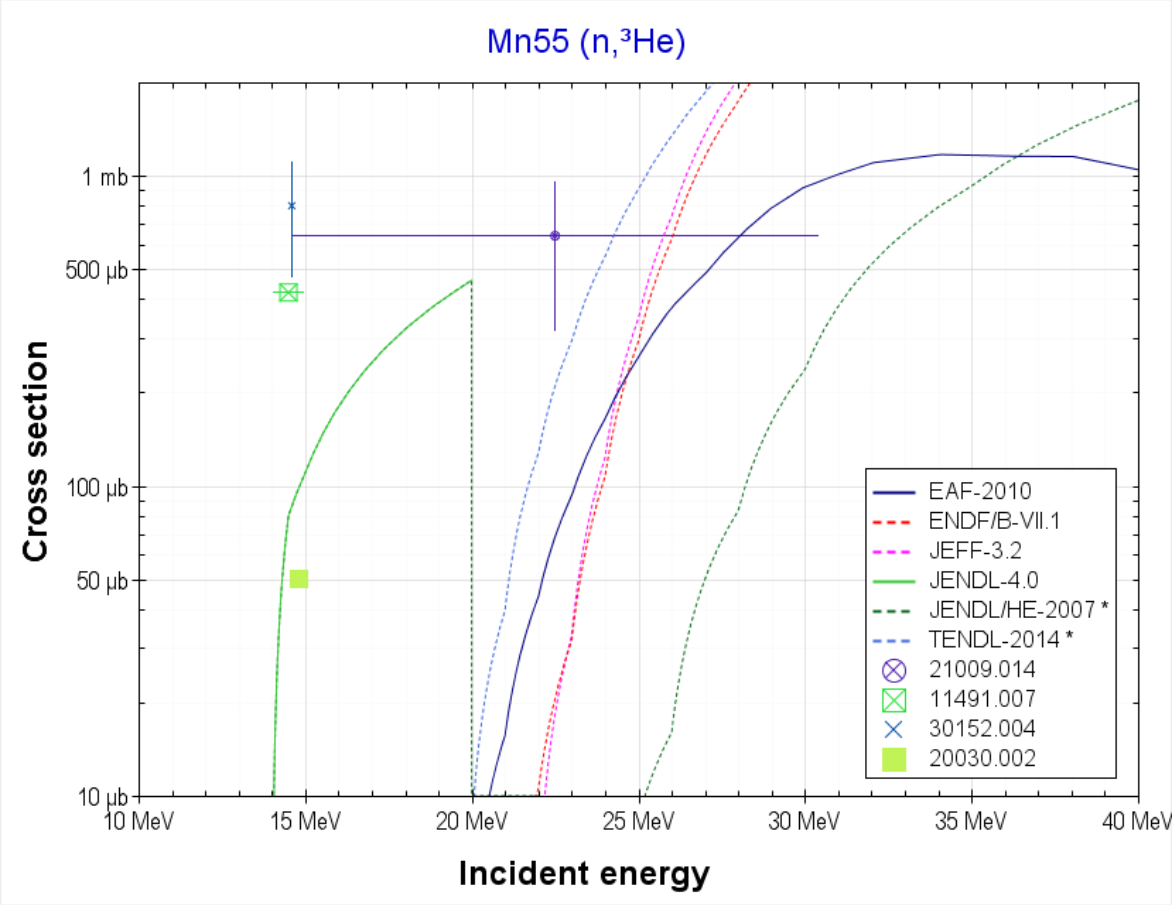
- **Figure.** Cu63 (n,He3)
- **Figure.** Mn55 (n,He3)

Figure. Cu63 (n,He3)



- EXFOR data, threshold reactions

Figure. Mn55 (n,He3)

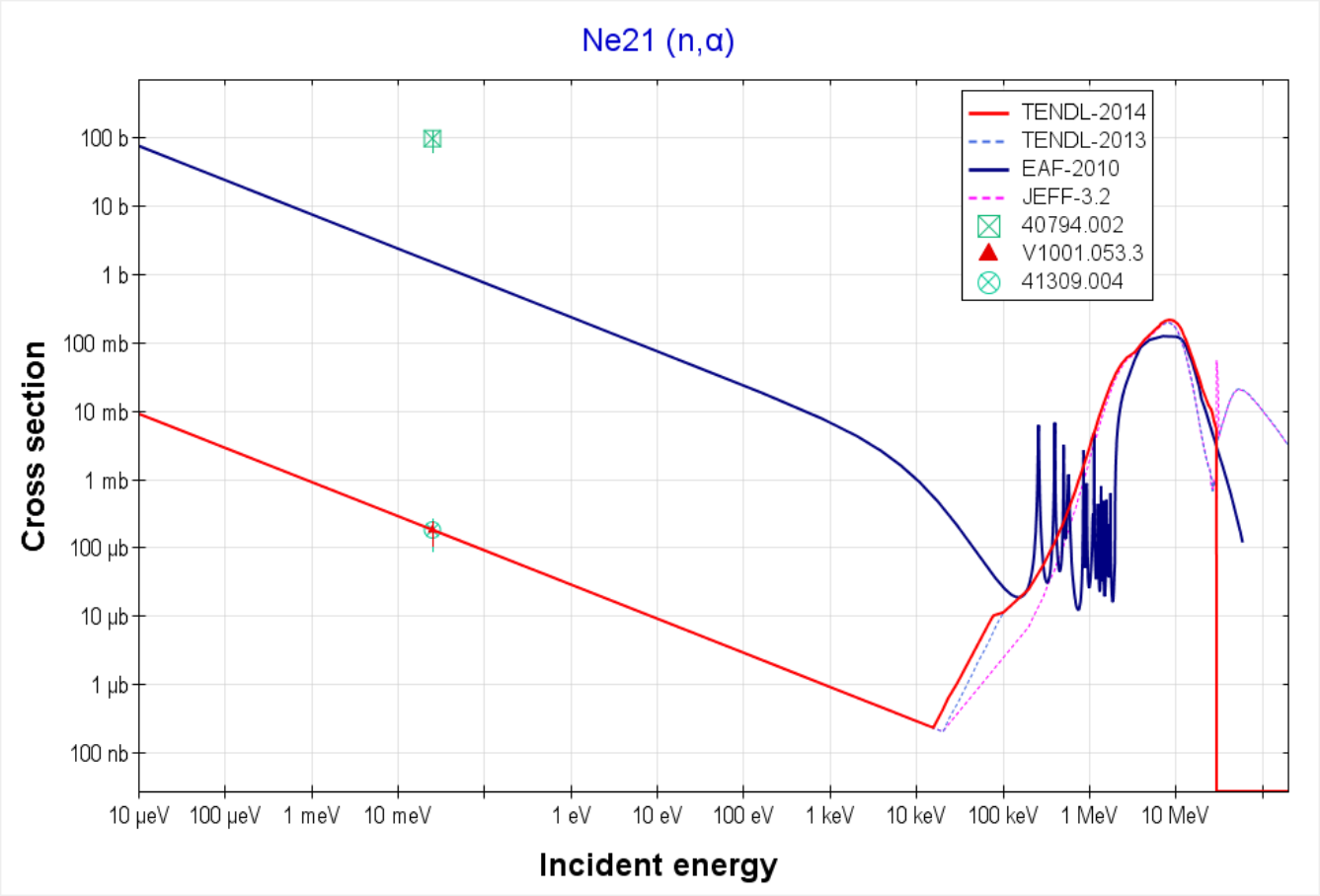


- EXFOR data, threshold reactions

Reactions (n,alpha)

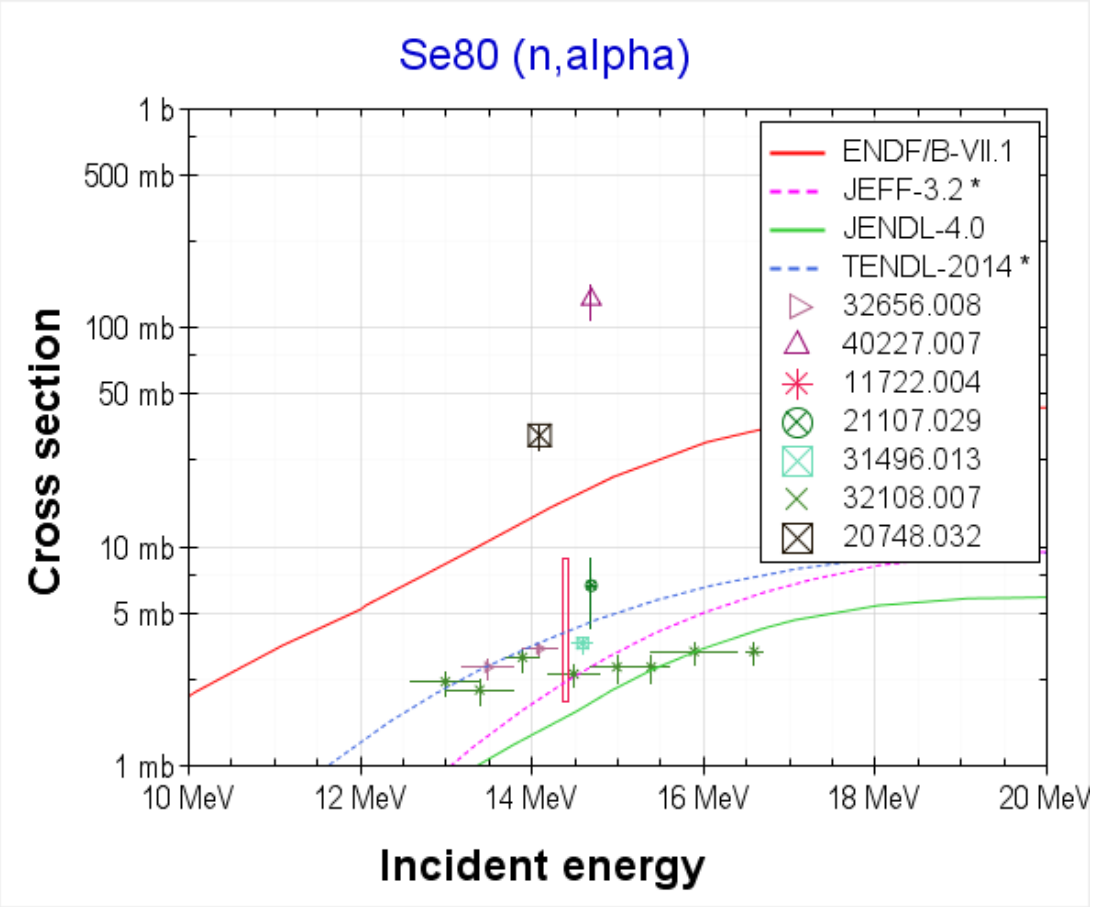
- **Figure.** Ne21(n,alpha) O18 rank value=1.47
- **Figure.** Se80 (n,alpha)
- **Figure.** Sc45 (n,alpha)
- **Figure.** Ge74 (n,alpha) Zn71-G

Figure. Ne21(n,alpha) O18 rank value=1.47



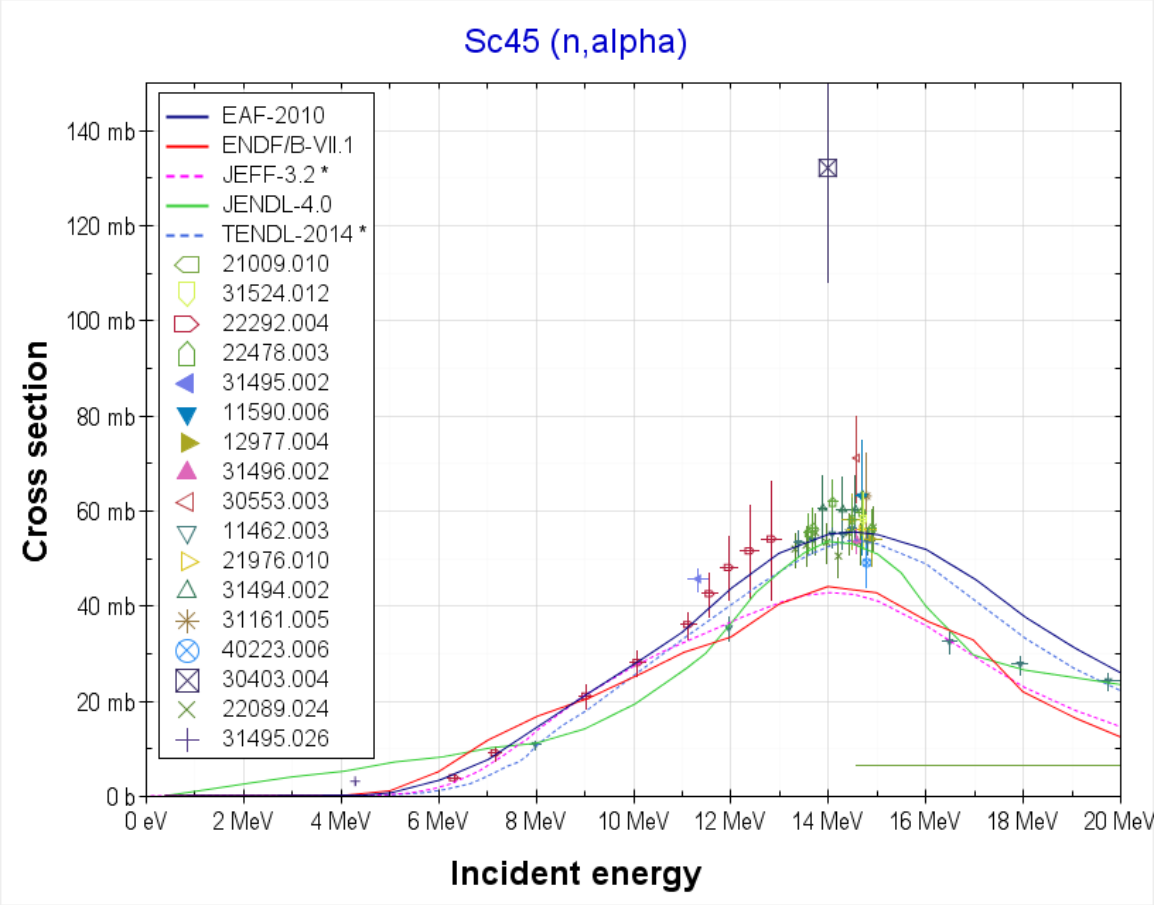
- EXFOR data to be discharged?

Figure. Se80 (n,alpha)



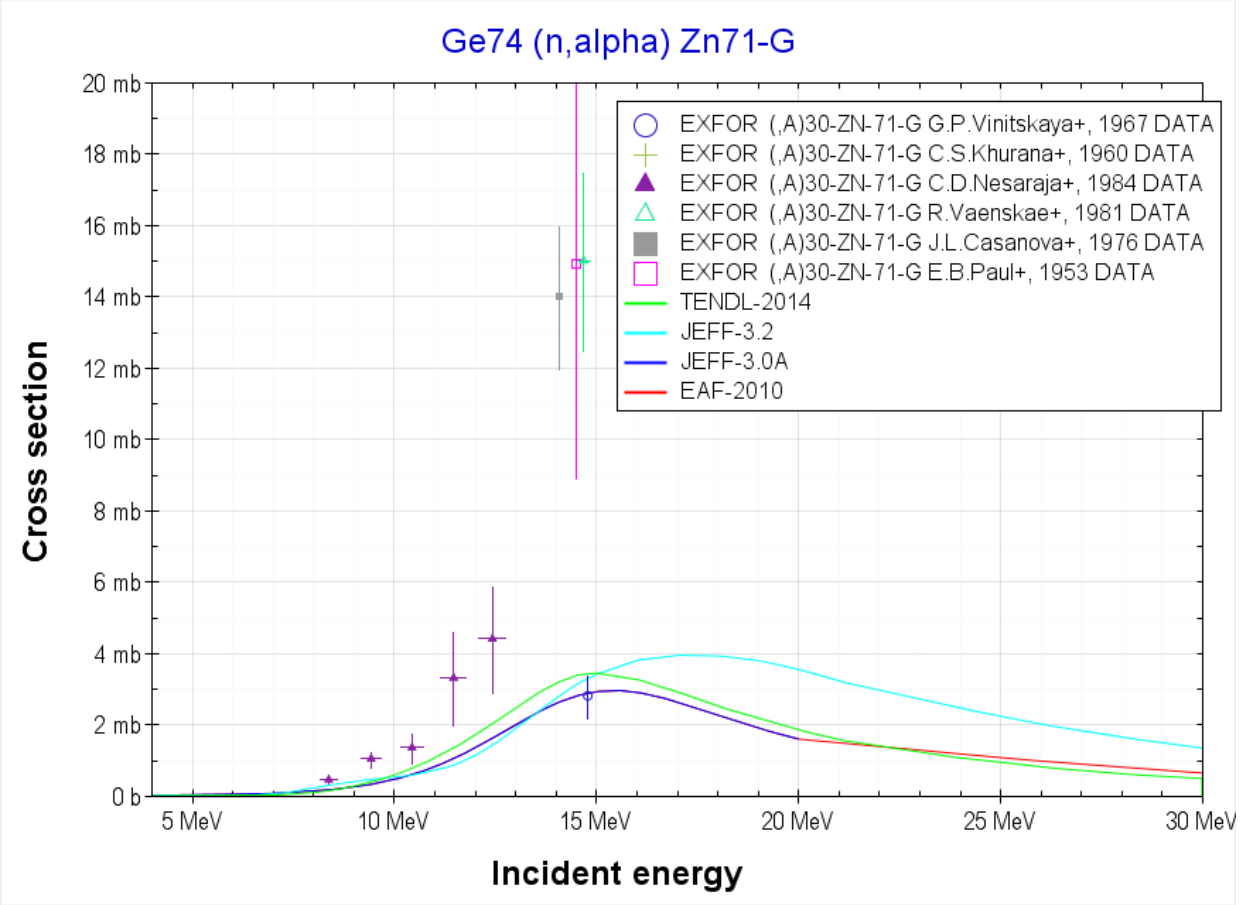
- EXFOR data to be checked

Figure. Sc45 (n,alpha)



- EXFOR data to be checked and/or discharged by evaluators

Figure. Ge74 (n,alpha) Zn71G

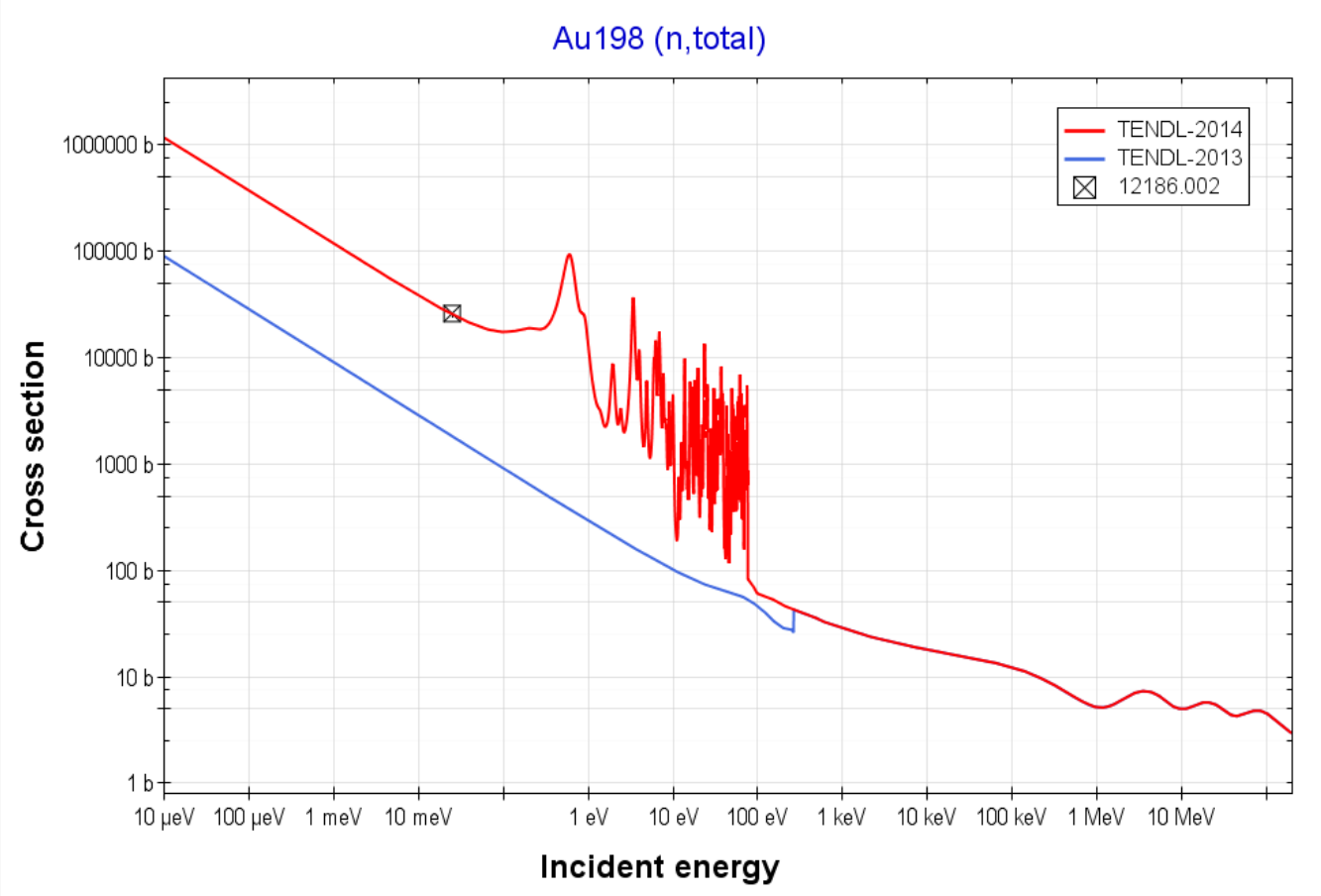


- EXFOR data to be checked for isomeric reactions!

Reactions (n,tot)

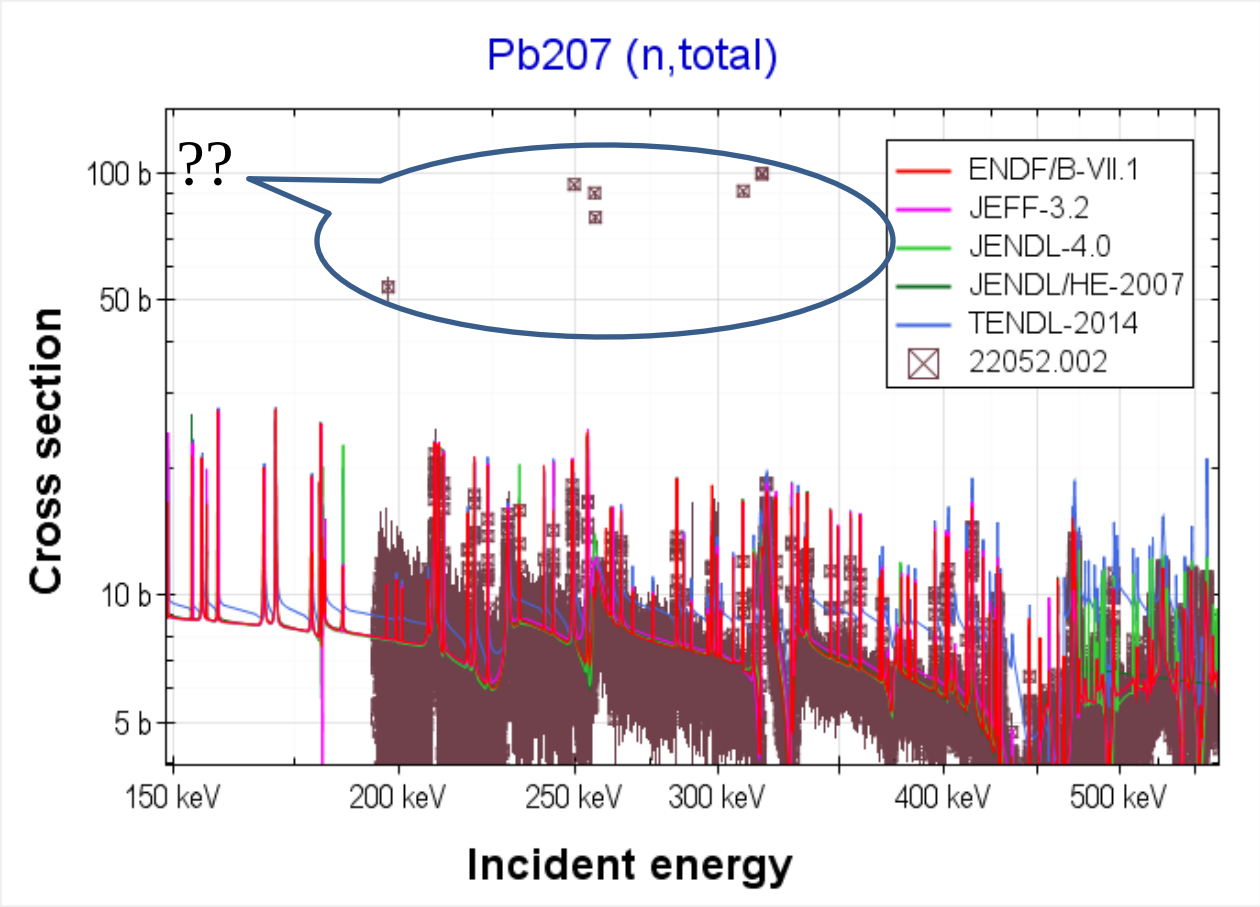
- **Figure.** Au198(n,tot) rank value=1.65
- **Figure.** Pb207(n,tot)

Figure. Au198(n,tot) rank value=1.65



- New evaluations (e.g.TENDL-2014)

Figure. Pb207(n,tot)



- EXFOR outliers in the same large ENTRY?

Thank you for your attention

References

- NEA (2011), “Statistical methods for the verification of databases”, *NEA News*, Volume 29, No. 1, OECD, Paris.

- NEA (2012), “NEA contributions to the worldwide collection, compilation and dissemination of nuclear reaction data”, *NEA News*, Volume 30, No. 2, OECD, Paris.

- Société de Calcul Mathématique (SCM) (2014), “Cross checking of large evaluated and experimental nuclear reaction databases”, International Conference on Nuclear Data for Science and Technology, *Nuclear Data Sheets*, Volume 120, pp. 277-280, Elsevier.

- NEA (2014), “Statistical verification and validation of the EXFOR database”, NEA Data Bank Report, NEA/DB/ DOC(2014)3, OECD, Paris.

- NEA (2014), “EXFOR: Improving the quality of international databases”, *NEA News*, Volume 32, No. 1, OECD, Paris. (E. Dupont). - **This presentation is mainly based on this work.**